Pentafluorobenzoic acid, propyl ester

Other names: Propyl pentafluorobenzoate
Inchi: InChI=1S/C10H7F5O2/c1-2-3-17-10(16)4-5(11)7(13)9(15)8(14)6(4)12/h2-3H2,1H3
InchiKey: QZYJMLLSDNHSOD-UHFFFAOYSA-N
Formula: C10H7F5O2
SMILES: CCCOC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 254.15
CAS: 97649-89-3

Physical Properties

Property code	Value	Unit	Source
gf	-1110.39	kJ/mol	Joback Method
hf	-1295.90	kJ/mol	Joback Method
hfus	31.94	kJ/mol	Joback Method
hvap	48.51	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	2.949		Crippen Method
mcvol	144.290	ml/mol	McGowan Method
pc	2265.42	kPa	Joback Method
rinpol	1134.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1126.00		NIST Webbook
ripol	1434.00		NIST Webbook
ripol	1426.00		NIST Webbook
ripol	1419.00		NIST Webbook
ripol	1460.00		NIST Webbook
ripol	1423.00		NIST Webbook
ripol	1460.00		NIST Webbook
ripol	1469.00		NIST Webbook
tb	552.42	K	Joback Method
tc	725.14	K	Joback Method
tf	366.59	K	Joback Method

vc	0.602	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.91	J/mol×K	552.42	Joback Method
cpg	349.36	J/mol×K	581.21	Joback Method
cpg	358.45	J/mol×K	609.99	Joback Method
cpg	367.17	J/mol×K	638.78	Joback Method
cpg	375.54	J/mol×K	667.56	Joback Method
cpg	383.53	J/mol×K	696.35	Joback Method
cpg	391.15	J/mol×K	725.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97649893&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume